Phenol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.58 days

Global applicability domain: Outside

Local applicability domain index: 3.77e-01

Confidence level: 6.98e-01

Nearest Neighbors from the Training Set

Image not found
Ethylcyclohexane
Measured: 4.93
Predicted: 3.02

Image not found
Ethylcyclopentane
Measured: 511
Predicted: 8.14

Image not found
Ethylbenzene
Measured: 120
Predicted: 6.21

Image not found
Toluene
Measured: 4.93
Predicted: 3.42

Image not found
Methylcyclopentane
Measured: 24.3
Predicted: 4.41